Low-Energy Linear Structures in Dense Oxygen: Implications for the ε-phase

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Oxygen is a dominant player in life sciences and technology, and there is still much to be known about its behavior. In solid form it exhibits remarkable complexity with increasing density: at first an insulating antiferromagnet, it actually becomes metallic and superconducting at high enough pressures and low enough temperatures.

Solid oxygen at high density is particularly striking for its puzzling 'red' or ε-phase, possessing strong infrared (IR) activity in two quite different frequency bands which apparently emanates from a structure that has been elusive to experimentalists for over two decades.

Using first-principles density functional theory we observe a symmetrical low-density phase to be unstable with increasing pressure to an unusual arrangement of linear chains, preserving a known tendency of the light elements toward linear structures (Fig. 1). The newly predicted structure exhibits many properties in striking agreement with experimental data, including the IR activity.

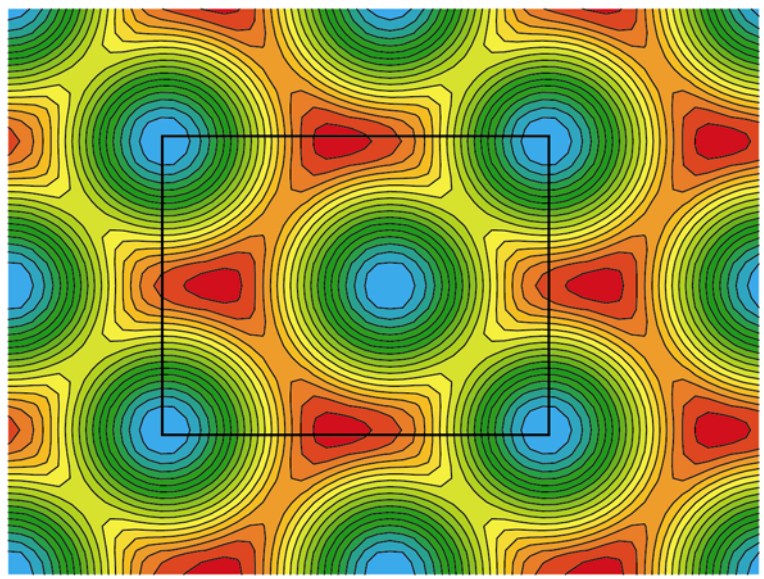

Fig. 1 Shown is the computed electronic charge density of a newly-predicted ground state structure at 200,000 atmospheres, illustrated by a section taken through the molecular centers and perpendicular to the molecular axes. (Blue is highest, red lowest, with the chains running top to bottom.) [Phys. Rev. Lett. **88**, 205503 (2002)]